

Nithiamide
140-40-9 | DTXSID6046391

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.41e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.82e-01

Confidence level: 4.90e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,3,7-Trichlorodibenzo-p-dioxin</div> <div>Measured: 2.00e-06</div> <div>Predicted: 1.72e-07</div>	<div>Image not found</div> <div>Nitric acid, hexyl ester</div> <div>Measured: 2.30e-04</div> <div>Predicted: 2.68</div>	<div>Image not found</div> <div>Orbencarb</div> <div>Measured: 2.00e-06</div> <div>Predicted: 1.81e-05</div>
<div>Image not found</div> <div>Aldicarb sulfoxide</div> <div>Measured: 9.00e-05</div> <div>Predicted: 6.19e-05</div>	<div>Image not found</div> <div>2-Methylfuran</div> <div>Measured: 1.20e-04</div> <div>Predicted: 66.8</div>	